International Journal of Quantum Chemistry Author Index—Volume 54

Adamowicz, L. See Zhang, Z., 281
Aoki, Y. See Mitani, M., 167
Aquino A., N.
Accurate Energy Eigenvalues for Enclosed Hydrogen Atom Within Spherical Impenetrable Boxes, 107
Averyanov, A. S. See Khait, Yu. G., 329

Bhattacharyya, K. See Pathak, R. K., 13
Bhattacharyya, S. P. See Sarkar, P., 337
Bian, W.
—; Deng, C.: Direct Solution of the Many-Body Schrödinger Equation in the Hyperspherical Formalism: Application of the CFHH–GLF Method to a Set of He-Like Systems, 273
Bochicchio, R. C.
—; Grinberg, H.: On Master Equations, Spectral Resolutions, and Self-Energy Fields in Propagator Theories for Quantum Open Systems, 27
—; See Ponec, R., 99
Botella, V. See Fernández-Serra, P., 305
Brändas, E. J.
Review of *The Physics of Atoms and Quanta: Introduction to Experiments and Theory*, 4th edition, by H. Haken and H. C. Wolf, 325
Bu, Y.
—; Zhang, Y.; Qiu, L.: Theoretical Studies on the Inner-Sphere Reorganization Energies for the Self-Exchange Reactions of Gas-Phase Diatomic Molecules HA (A = Mg, Al, Si, P, S, Cl), 249

Calais, J. L.
See Jürimäe, T., 369
Calamante, F.
—; Grinberg, H.: Padé Approximants to the Evolution Operator Through the Lippmann Schwinger Variational Principle, 137
Cao, Y.
—; Chen, L.; Chen, B.; Fen, J.; Chen, W.; Pan, Y.-K.: Band Structure Studies on Crystalline C_{60}, Ca_3C_{60}, and Ca_5C_{60}, 265
Cassam-Chenaï, P.
Ensemble Representable Densities for Atoms and Molecules. I. General Theory, 201
Chen, B. See Cao, Y., 265
Chen, L. See Cao, Y., 265
Chen, N.-Y. See Liu, H.-L., 89
Chen, W. See Cao, Y., 265
Chu, S.-Y. See Su, Y.-N., 43
Coleman, A. J.
—; Yukalova, E. P.; Yukalov, V. I.: Pairon Distributions and the Spectra of Reduced Hamiltonians, 211
Cruz, S. A.
—; Ley-Koo, E.; Marín, J. L.; Taylor-Armitage, A.: Variational Calculations for the Hydrogen Atom Confined in Spaces with Paraboloidal and Spheroidal Boundaries, 3

Datta, S. N. See Mallik, B., 271
Davidson, E. R. See Ju, G.-Z., 299
Delgado-Barrio, G. See Fernández-Serra, P., 305
Deng, C. See Bian, W., 273

Fang, J.-Y.
—; Thomson, C.: Hydrogen-Bonding Effects, Electrostatic Potential, and the Antitumor Activity of Flavone Acetic Acid and Related Compounds. I. Ab Initio Studies on the First Stable Conformations, 313
Fen, J. See Cao, Y., 265
Fernández-Serra, P.
— Botella, V.; Smeyers, Y. G.; Galano, A.; Delgado-Barrio, G.: Ground-State and Some Excited States of Li_2 By the Half-Projected Hartree–Fock Method, 305
Frisch, M. J. See Schlegel, H. B., 83

Galano, A. See Fernández-Serra, P., 305
Grinberg, H. See Calamante, F., 137
—; See Bochicchio, R. C., 27
Guenzburger, D. See Nogueira, S. R., 381
Guseinov, I. I.
—; Yassen, R. F.: Unified Treatment of Two-Center Coulomb, Hybrid, and Exchange Integrals over Slater-Type Orbitals, 197

Hall, G. G. See Rees, D., 351
—; See Rees, D., 361
Hertwig, R. H.
—; Holthausen, M. C.; Koch, W.; Maksić, Z. B.: Ab Initio MO and Approximate Density Functional Theory Studies on the Lowest Singlet and Triplet States of *s*- and *as*-Indacene, 147
Holthausen, M. C. See Hertwig, R. H., 147

Igawa, A.
A Method of Calculations of the Matrix Elements Between the Spin-Projected Nonorthogonal Slater Determinants, 235
Imamura, A. See Mitani, M., 167

Jansen, A. P. J. See Teunissen, E. H., 73
Jaskólski, W. See Zicovich-Wilson, C., 61
Ju, G.-Z.
—; Machado, F. B. C.; Davidson, E. R.: On Electron Correlation in $NaCl_2$, 299

Jürimäe, T.
—; Strandberg, M.; Karelson, M.; Calais, J. L.: A Semiempirical Study of Heterocycle Oligomers and Polymers in Different Dielectric Media, 369
Jursic, B. S.
—; Zdravkovski, Z.: Theoretical Investigation of *cis*- and *trans*-Nitric Oxide Dimers with Ab Initio and Density Functional Gaussian-Type Orbital Approach, 161

Karelson, M. See Jürimäe, T., 369
Kato, H. See Nakajima, Y., 51
Khait, Yu. G.
—; Panin, A. I.; Averyanov, A. S.: Search for Stationary Points of Arbitrary Index by Augmented Hessian Method, 329
Koch, W. See Hertwig, R. H., 147
Koga, T.
—; Watanabe, S.; Thakkar, A. J.: Numerical Hartree–Fock Results for Atoms Cs Through Lr, 261

Ladik, J. J. See Liu, H.-L., 89
Lagowski, J. B. See Raja, A. V., 117
Ley-Koo, E. See Cruz, S. A., 3
Li, Y.-M.
—; Xiao, H. M.: Studies on the Mechanism of Mannich Reaction Involving Iminium Salt as Potential Mannich Reagent. III. Furan as Pseudo Acid Component, 293
Liu, H.-L.
—; Chen, N.-Y.; Ladik, J. J.; Otto, P.: A New Boundary Treatment: HF Surface Potential Model Applied to Solid-State Cluster Calculations, 89
Löwdin, P.-O.
International Journal of Quantum Chemistry—A Journal Devoted to Quantum Theory and Computations in Chemistry, Condensed Matter Physics, and Biology, 1
Luo, L.
Conformation-Transitional Rate in Protein Folding, 243

Machado, F. B. C. See Ju, G.-Z., 299
Maksić, Z. B. See Hertwig, R. H., 147
Mallik, B.
—; Datta, S. N.: Erratum to "Semiempirical Quantum Chemical Treatment of the Standard Reduction Potentials of Quinone and Plastoquinone in Water", 271
Marín, J. L. See Cruz, S. A., 3
Mitani, M.
—; Aoki, Y.; Imamura, A.: Electronic Structures of Large, Extended, Nonperiodic Systems by Using the Elongation Method: Model Calculations for the Cluster Series of a Polymer and the Molecular Stacking on a Surface, 167

Nakajima, Y.
—; Sakagishi, Y.; Shiibashi, M.; Suzuki, Y.; Kato, H.: A PM3 Study on Intrinsic Decarboxylation Process of Methyl–Ethyl–α–Pyridylacetic Acid, 51
Nogueira, S. R.
—; Guenzburger, D.: Electric-Field Gradients and Magnetic Hyperfine Parameters of Square-Pyramidal $[M(CN)_5]^{3-}$ (M = Co, Rh, and Ir) Complexes, 381

Otto, P. See Liu, H.-L., 89

Packer, M. J.
—; Pickup, B. T.: An Analysis of Dynamic Linear Response Properties at RPA Level, 223
Palting, P.
On Weak and Strong Conjugacy in the Antisymmetry Principle, 19
Pan, Y.-K. See Cao, Y., 265
Panin, A. I. See Khait, Yu. G., 329
Pathak, R. K.
—; Bhattacharyya, K.: Eigenstates of Double Wells at Varying Wells Depths, 13
Pickup, B. T. See Packer, M. J., 223
Planelles, J. See Zicovich-Wilson, C., 61
Polášek, M.
—; Zahradník, R.: A Quantum Chemical Study of Small Beryllium Hydrides and Their Radical Anions, 93
Ponec, R.
—; Bochicchio, R. C.: Nonlinear Population Analysis From Geminal Expansion of Pair Densities, 99

Qiu, L. See Bu, Y., 249

Raja, A. V.
—; Lagowski, J. B.: Conformational Study of Halogen- and Hydrogen-Substituted Polythionylphosphazenes Using Density Functional Theory Method, 117
Rees, D.
—; Hall, G. G.: Localized Functions on a Circle, 351
—; Hall, G. G.: Localized Planar Atomic Hybrids, 361

Sakagishi, Y. See Nakajima, Y., 51
Sarkar, P.
—; Bhattacharyya, S. P.: The Effects of Static Quartic Anharmonicity on the Quantum Dynamics of a Linear Oscillator with Time-Dependent Harmonic Frequency: Perturbative Analysis and Numerical Calculations, 337
Schlegel, H. B.
—; Frisch, M. J.: Transformation Between Cartesian and Pure Spherical Harmonic Gaussians, 83
Shiibashi, M. See Nakajima, Y., 51
Smeyers, Y. G. See Fernández-Serra, P., 305

Strandberg, M. See Jürimäe, T., 369
Su, Y.-N.
—; Chu, S.-Y.: Structure and Bonding Study of the $P_2 + P_2^+$ System, 43
Suzuki, Y. See Nakajima, Y., 51

Taylor-Armitage, A. See Cruz, S. A., 3
Teunissen, E. H.
—; Jansen, A. P. J.: Large Basis Sets and Geometry Optimizations in Embedded Cluster Calculations, 73
Thakkar, A. J. See Koga, T., 261
Thomson, C. See Fang, J.-Y., 313

Watanabe, S. See Koga, T., 261

Xiao, H. M. See Li, Y. M., 293

Yassen, R. F. See Guseinov, I. I., 197
Yukalov, V. I. See Coleman, A. J., 211
Yukalova, E. P. See Coleman, A. J., 211

Zahradník, R. See Polášek, M., 93
Zdravkovski, Z. See Jursic, B. S., 161
Zhang, Y. See Bu, Y., 249
Zhang, Z.
—; Adamowicz, L.: Newton–Raphson Optimization of the Explicitly Correlated Gaussian Functions for the Ground State of the Beryllium Atom, 281
Zicovich-Wilson, C.
—; Jaskólski, W.; Planelles, J.: Atoms and Molecules in Cavities: A Method for Study of Spatial Confinement Effects, 61

International Journal of Quantum Chemistry Subject Index—Volume 54

Ab initio Hartree–Fock self-consistent-field MO method, 249
Ab initio MO method, 147
Ab initio calculations, 43, 93
Ab initio methods, 161
Ab initio molecular densities, 201
Ab initio molecular orbital (MO) theory, 117
Alias functions, 351, 361
Anions, 93
Antisymmetry principle, 19
Antitumor activity, 313
Approximate density functional method *s*-indacene, 147
Arbitrary fixed index, 329
as-indacene, 147
Aufbau chain, 19
Augmented Hessian (AH) method, 329

Band structure, 265
Basis set, 73
Basis-set effects, 313
Basis-set quantum chemical calculations, 61
Beryllium atom, 281
Beryllium hydrides, 93
Bonding, 43
Boundary treatment, 89

Cartesian Gaussians, 83
CFHH–GLE method, 273
cis-NO dimer, 161
Cluster-series calculations, 167
Commuting matrices, 351, 361
Complex exponentials, 351
Conformational analysis, 117
Conformational transition, 243
Conjugacy, 19
Coulombian potential, 107
Crystal orbitals, 265

Decarboxylation, 51
Density functional self-consistent spin-polarized calculation, 381
Density functional theory (DFT), 117
Density functional theory methods, 161
Discrete variational method, 381
Dissociation energies, 43
Double-well potentials (DWP), 13
Dynamic linear response, 223

Eigenenergies, 13
Eigenstates, 13
Electron correlation, 299, 305
Electron-interaction contributions, 223
Electron paramagnetic resonance, 381
Elongation method, 167
Embedded cluster method, 73
Enclosed hydrogen atom, 107
Energy eigenvalues, 107
Ensemble representable densities, 201
Evolution operator, 137
Explicitly correlated Gaussian functions, 281

Fermi interaction, 381
Fermionic wave function, 201
Finite basis, 351, 361

Gas-phase electron-transfer processes, 249
Gaussian functions, 281
Geminal expansion, 99
Generalized Laguerre function (GLF), 273
Geometry optimizations, 73
Ground states, 261, 265

Half-projected Hartree–Fock wave function (HPHF), 305
Harmonic frequency (ω), 337
Hartree–Fock (HF) surface potential model, 89
He-like systems, 273
Heavy atoms, 261
Hermitian Hamiltonians, 137
Heterocycles, 369
Hydrogen atom, 3
Hydrogen-bonding effects, 313
Hyperspherical harmonics (HH), 273

Infinite potential, 107
Inner-sphere reorganization energies (RE), 249
Interpair correlation energy, 299
Intrapair correlation energy, 299

LCAO–MO–SCF ab initio method, 89
Linear oscillator, 337
Lippmann Schwinger variational principle, 137
Localized atomic hybrids, 361
Localized equivalent functions, 351

Mannich reactions, 293
Mannich reagent, 293
Master equations, 27
Matrix elements, 235
Methyl–ethyl–α pyridylacetic acid (MEPA), 51
Microscopic cavity, 61
MNDO–PM3 method, 51
Model space approximation, 61
Molecular dipole moment, 361
Molecular electrostatic potential, 313
Molecular stacking, 167
MP2 (geometries), 93
MP4 (energies), 93

Neumann expansion, 197
Newton–Raphson optimization, 281
NO monomer, 161
Nonadiabaticity operator method, 243
Nonlinear population analysis, 99
N-particle problem, 211
Numerical Hartree–Fock (NHF) computations, 261

Oligomers, 369
One-electron contribution, 223

$P_2 + P_2^+$ system, 43
Padé approximants (PA), 137
Pair densities, 99
Pair energies, 299
Pairon distribution, 211
Paraboloidal boundaries, 3
Paramagnetic complexes, 381
Point-group symmetry, 89
Polymers, 369

Polythionylphosphazenes, 117
Propagators, 27
Protein folding, 243

Quantum dynamics, 337
Quantum open systems, 27
Quartic anharmonicity, 337

Reduced Hamiltonian, 211
Resonating Hartree–Fock (Res HF) approximation, 235
RPA equation, 223

Self-consistent reaction field theory in the multicavity approximation (MCa SCRF), 369
Self-energy fields, 27
Semiempirical AM1 quantum mechanical method, 293
Semiempirical MNDO calculations, 99
Semiempirical PM3 parameterization, 369
Simultaneous eigenfunctions, 351, 361
Slater determinants, 305
Slater-type orbitals, 197
Solid-state cluster calculations, 89
Spherical harmonic Gaussians, 83
Spherical impenetrable boxes, 107
Spheroidal boundaries, 3
Spin-projected nonorthogonal Slater determinants (S dets), 235
Square-pyramidal geometry, 381
Stationary points, 329

Three-body Schrödinger equation, 273
Three-dimensional EHMO crystal orbital calculations, 265
Time-dependent force constant (K), 337
Time-dependent Fourier grid Hamiltonian method, 337
Transformation coefficients, 83
trans-NO dimer, 161
Two-center Coulomb integrals, 197
Two-center exchange integrals, 197
Two-center hybrid integrals, 197
Two-electron contribution, 223